

## **A Priori Prediction of Pure Component and Mixture Properties using COSMO-RS**

O. Spuhl S

*Institut fuer Verfahrenstechnik, FG Thermodynamik und Thermische Verfahrenstechnik, Technische Universität Berlin, Berlin, Germany*

W. Arlt C

*Institut fuer Verfahrenstechnik, FG Thermodynamik und Thermische Verfahrenstechnik, Technische Universität Berlin, Berlin, Germany*

Predicting thermodynamic properties is still challenging for chemical engineers. The COSMO-RS model developed by A. Klamt has shown promising results applied to mixtures of polar and non-polar substances like hydrocarbons, alcohols, ethers and ketones. There it was used as a gE model describing the reality of the liquid phase by using its ability to predict the activity coefficient of a component in mixture. COSMO-RS determines molecular interactions on the basis of quantum-chemistry calculations and calculates the chemical potential of a component using a statistical mechanics approach. Still the characterization of pure component properties with COSMO-RS is below acceptable accuracy, in particular when it is applied to the prediction of vapor pressures. Here we will present a new approach to extend the energy concept of COSMO-RS. The change in Gibbs enthalpy when a molecule is transported from the vapor phase into the liquid phase was not precisely taken into account within the original COSMO-RS concept. It was described as the energy difference by moving a molecule from the vacuum into an ideal screened conductor, the reference state in the COSMO-RS model. We replace that term using the Scaled-Particle-Theory which is known to be able to model the insertion of a hard-sphere into a hard-sphere fluid. The application of this theory leads to an expression which gives the partial molar Gibbs enthalpy of a component  $i$  in the solvent S caused by forming a cavity for the sphere and establishing repulsive interactions with the surrounding particles. This enables us also to replace the rather empirical combinatorial term of COSMO-RS. Combining the existent energy terms, i.e. dispersive and electrostatic energies, with the new one gives an extended more reasonable energy concept. This concept is applied to small hydrocarbons and alcohols which can be approximated by a spherical particle. Results for the prediction of the vapor pressure are presented. The capability of improved prediction of binary vapor-liquid phase equilibria considering mixtures of hydrocarbons and alcohols is also shown.